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NIST Technical Note 1403

Chaos, Dissipation, Arrow of Time, in Quantum Physics

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#1403
1993

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May 1993

U.S. Department of Commerce
Ronald H. Brown, Secretary

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National Institute of Standards
and Technology
Technical Note 1403
Nati. Inst. Stand. Technol.
Tech. Note 1403
12 pages (May 1993)
CODEN: NTNOEF

U.S. Government Printing Office
Washington: 1993

For sale by the Superintendent
of Documents
U.S. Government Printing Office
Washington, DC 20402

CHAOS, DISSIPATION, ARROW OF TIME, IN QUANTUM PHYSICS

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Abstract

A compact description of the evolution of a many-body system, e.g., a dilute gas, is provided by the generalization of the usual reaction S-matrix or U-matrix to a system S- or U-matrix. Using this tool it is demonstrated, that (i) the characterization of quantum chaos turns out to be very transparent: already exceedingly simple systems, including time-reversal invariant states, are capable of exhibiting quantum chaos; (ii) the time-reversal invariance of the Hamiltonian leads to relaxation of arbitrary non-equilibrium states of chaotic quantum systems, i.e., to dissipation, which thus allows the definition of a quantum arrow of time; (iii) the second law of thermodynamics, and hence the complete field of thermodynamics, is a consequence of quantum physics.

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1 Introduction

The question of chaos, in particular also of quantum chaos, over the last few years has attracted considerable attention. Surprising as its recognition was, the existence of mathematical chaos, or as it also is called, deterministic chaos, does not offer conceptual paradoxes. This is not immediately so for quantum chaos, and for classical chaos – which, being the limit for large quantum numbers of quantum chaos, should be distinguished from mathematical chaos which has inherently infinite precision. To wit, the term "chaos" implies in some sense unpredictability and irreversibility of the motion of the system; sometimes it is expressed as "high sensitivity to initial conditions." A conceptual difficulty in searching for chaos in quantum physics arises from the fact that the motion of the system is governed by a Hamiltonian which is time-reversal invariant, and that the spectrum of the system is discrete, or actually must be discretized in order to achieve localizability of the system components. Time-reversal invariance and chaos on the face of it seem contradictory. Because of the time-reversal invariance of the Hamiltonian non-chaotic time-reversal invariant states must actually exist. One of our tasks will be to identify those states. The aim of this short note is to clear up these points and to briefly indicate their consequences. To that end, in section 2, by studying the time evolution of a quantum system we will give a description of the essence of quantum chaos, and a simple mathematical criterion for its identification. Furthermore, we will demonstrate that in quantum physics only exceptional systems do not exhibit the character of chaos, and that it is essentially impossible, i.e., only in an un-real, idealized manner possible, to construct such states. This will set the stage for the understanding of the mechanism of dissipation in quantum physics, which is the subject of the following section.

One of the important points we shall demonstrate is that a chaotic quantum system undergoes relaxation, i.e., it exhibits the effect of dissipation, simply as the consequence of its evolution being governed by quantum dynamics. This will be done in section 3. Of course, being part of quantum physics, the description of the evolution allows the treatment of arbitrarily off-equilibrium situations. More precisely, as we will see, the system evolves towards equal occupation probability for the accessible phase space cells. This way the basic axiom of statistical thermodynamics, *viz.*, the assumption of equal *a priori* probability for the occupation of the phase space cells at thermal equilibrium, turns out to be a consequence of the quantum physics evolution. Hence, all results of statistical thermodynamics turn out to be correct; in particular, the second law of thermodynamics is fulfilled. More broadly, the whole field of thermodynamics thus turns out to be a consequence of the dynamics in quantum physics. At the same time the entropy can be used to define the quantum physics arrow of time in non-equilibrium systems.

The broader question of the thermodynamic variables will be addressed in a separate paper.

2 Time-Reversal Invariant States

Since the Hamiltonian (by assumption!) is time-reversal invariant then for any solution of the equations of motion, say $\psi(t)$, the time-reversed state, $\phi(t) = \psi(-t)^*$, is also a solution. Consequently

$$\Psi(t) = \psi(t) \; + \; \phi(t) \quad , \tag{1}$$

which is time-reversal invariant, is also a solution. Our first task is to identify the time-reversal invariant states; then we will show that they do not exist in nature and why. To that end, we shall first consider the evolution in time of a two-body collision, and then that of a dilute gas.

The prototype elastic two-body scattering system at energy E is described as consisting in the asymptotic region of an incoming plane wave and an outgoing spherical wave. This description has two related difficulties: the waves fill all space and generate unphysical interference patterns; and there is no before or after the collision, they collide all the time [1]. The system is delocalized in space and time. To avoid these difficulties we shall employ the Weyl eigendifferential states which are defined as [2]

$$\Psi_W(E_k) = \mathcal{N} \int_{E_k-\epsilon}^{E_k+\epsilon} dE\ \Psi(E) \tag{2}$$

where $\epsilon \to 0$ is understood and $\mathcal{N}$ is the normalization constant. Furthermore, $\Psi(E)$ is the complete system wave function, i.e., it includes all channels and the actual collision region.

The Weyl states have several useful characteristics: (a) they are as close to being eigenstates of the Hamiltonian as can be while being localized in space and time; for large negative t the colliding systems in a "physical" scattering state are far apart and are approaching each other; at $t = 0$ they collide; and at positive t the reaction products fly apart; (b) the original continuous spectrum has been discretized, i.e., the number of Weyl states is denumerably infinite and thus only summations and not integrations are encountered: they are Kronecker orthonormal; (c) in contrast to the Gaussian wave packets of the Wigner representation they have simple mathematical properties; (d) they are minimum-uncertainty wave packets and can be directly used to define the phase space cells: when replacing in the wave function Ψ the time t by $t - t_l$, then in the classification of phase space the indices k and l of Eq (2) play the roles of the commonly used coordinates p and q, respectively. When mentioning phase space cells it will be tacitly assumed that this has been done. Also, we will be able to achieve all our results using the Weyl wave functions, which represent pure states. We will not need the more general description by density matrices which would be needed if impure states were required [3].

We will conduct our discussions by first considering the individual sharp energy components, $\Psi(E)$ of Eq. (2), and then investigate the modifications resulting from the Weyl superposition according to Eq. (2). Thus, for example, a time-reversal invariant physical Weyl scattering state, constructed according to Eq. (1), therefore, at $t \ll 0$ would have in addition to the original incoming state in the "input channel," in which the colliding particles approach each other, also the time-reversed original outgoing state, i.e., particles in the original "output channels," approaching each other, all of them to meet at $t = 0$ at the origin. All these components must be phase-related.

When using Weyl states the description of the evolution of the state in the interaction picture presents no problems as at $t = -\infty$ the collision partners are infinitely far apart and do not interact; i.e., the system can be described by asymptotic states. This way, for example, the inner structure (e.g., the self-energy) of each of the colliding partners can be computed without the interference by the other partner. Hence, given the initial state in terms of the asymptotic states, i.e., the states which are the solutions of the channel Hamiltonians, then the final state, again in terms of the asymptotic states, is computed exactly by multiplying the state vector of the initial state by the S-matrix; or by the U-matrix if the starting point is at some finite time [4]. The difference between these two forms is that the U-matrix contains the closed channels,

i.e., the channels which contain off-the-mass-shell particles, while the S-matrix ignores them. Since the closed channels decrease in amplitude exponentially as the systems move apart, the difference between the U- and the S-matrix is important only very close to the actual collision. For brevity we shall always speak of the S-matrix, with the proviso that if need be one should use the U-matrix.

We will conduct the discussion in the asymptotic state representation. We describe the evolution of the system in time by following the evolution of some given initial state; that state may be known as the result of the system having been suitably prepared, or it may be a member of the (unknown) density matrix of the system. In case the energy of the two-body collision is above the inelastic threshold, the S-matrix is N by N, with $N > 1$; when including the photon channels, and describing the photon states by Weyl functions, N is denumerably infinite at any energy. For simplicity we ignore the photon channels; then N is some finite number, depending on the energy E of the collision (dropping the subscript k of Eq. (2) for brevity). The asymptotic states then can be classified according to the number of (elementary or composite) particles they contain.

For the discussion it is convenient to describe the channel states in hyperspherical coordinates [5] which contain only one radial coordinate. Consequently, omitting the angular parts, then for a given state, $\Psi(E)$ all channels, c, asymptotically for $r_c \to \infty$ have the form

$$\psi_c \;=\; a_c\, e^{i(k_c r_c - E_c t)} \;-\; b_c\, e^{-i(k_c r_c + E_c t)} \quad . \tag{3}$$

Here a_c is the amplitude "before," and b_c "after" the collision. In general these states have $|a_c| \neq |b_c|$, i.e., the in-current is not equal to the out-current; thus, they are not time-reversal invariant. In a "physical state" a_c exists in one channel, the incoming channel, b_c in all channels. Of course, owing to the time-reversal invariance of the Hamiltonian, the time-reversed state of any of those solutions is also a solution. There do exist time-reversal invariant states, *viz.*, the eigenchannel states [6], which are the eigenstates of the S- matrix. There exist N such states. Since the eigenchannel states form a complete set of states, any state, for example, a physical scattering state, can be written as a superposition of eigenchannel states. In general, all N eigenchannel states are needed for this superposition. A system which is in a pure eigenchannel state "before" the scattering event remains unscathed, i.e., is unchanged by the scattering process. For these states there holds

$$b_{c,n} \;=\; a_{c,n}\, e^{2i\eta_n} \quad . \tag{4}$$

(The S-matrix being unitary, it must have eigenvalues of absolute value 1; hence the eigenvalues, $e^{2i\eta_n}$, as written in Eq. (4), must have real eigenphases η_n.) Thus, the channel functions of an eigenchannel state are of the form (still in hyperspherical coordinates)

$$\psi_{c,n} \;=\; a_{c,n}\, e^{-i(E_c t + \eta_n)}\, \sin(k_c r_c - \eta_n) \quad ; \tag{5}$$

they have standing waves in all channels c, which evidently is necessary for time-reversal invariance, and which are phase-related. (Of course, a 1 by 1 S-matrix has only 1 channel, which is thus an eigenchannel.) The eigenchannel states are the only stationary time-reversal invariant states. In principle, even if not in practice, such states can be constructed. These states are delocalized continuum states. The Weyl eigenchannel states for $t \ll 0$ have phase-related incoming particles in all channels which collide at $t = 0$ and fly apart for $t \gg 0$, maintaining the relative amplitudes and the relative phases in the sense that η_n before the collision goes into $-\eta_n$ after the collision.

A physical state – which has an incoming wave in one channel and outgoing waves in all channels – is not time-reversal invariant. Again, the time-reversed state with incoming waves in all channels, outgoing wave in one channel, is also a possible solution. This time-reversed state then can be used to construct a time-reversal invariant state according to the prescription of Eq. (1). However, see below.

In a certain, somewhat inaccurate way, there exists a system which in some sense is an eigenchannel state. That case is given by the system which at the considered energy allows only elastic s-wave scattering. Then indeed the s-wave part of the wave function is described by a 1 by 1 S-matrix and has the form (5), i.e., it is in the time-reversal invariant form. However, the other multipolarities in the incoming plane wave remain in the time-reversal non-invariant superposition of a modified plane wave having the original direction of propagation. A convergent pure spherical s-wave has not yet been achieved in the laboratory.

Before continuing the discussion of the quantum physics system it may be informative to recall the case of a classical system. There exist exceptional systems which have closed trajectories in phase space. They almost by definition are in the non-chaotic regime; hence such systems must be "small." In a chaotic system the closed trajectories have measure zero; this statement actually defines a chaotic system. It is a different, but equivalent, form of the usual statement that chaotic motion is exponentially sensitive to the initial conditions. For the exceptional closed trajectory systems the entropy remains constant. All such systems are idealizations and not realizable in nature.

We now return to the quantum system. There the observation, equivalent to the above measure zero, is that the eigenchannel states (and also the time-reversed physical states) are represented by solutions which are unstable in the mathematical sense. Consider a given physical scattering state. Its exact time reversed state has an outgoing wave in exactly one channel. This situation is, however, mathematically unstable, in that a change of the amplitude even for only one of the incoming waves will generate a solution containing outgoing waves in all channels. (This change of the amplitude can be thought of as the addition of a physical state which has its incoming wave in that channel. This then results in outgoing waves in all channels.) In the same way, changing the amplitude only in one channel in an eigenchannel solution will unbalance the in- versus the out-currents in all channels.

This simple fact has dramatic consequences for a many-body system as we now will explain. We take the case of a dilute ideal gas in a mathematically perfect box, where the molecules are described by Weyl states in the asymptotic state representation. To describe the evolution of this system it is useful to introduce the system U-matrix; it is defined similarly as the usual U-matrix in terms of the Tomonaga-Schwinger equation [4], where the interaction picture interaction is the sum of the individual interactions between the collision partners. It is a generalization of the familiar graph expansion methods of many-body theory [7]. A more detailed discussion will be given in a separate paper. The restriction to a dilute gas leads to a substantial simplification and to conceptual transparency of the problem since then the evolution of the system can be treated in terms of the cluster expansion, which can be visualized as a sequence of 2- or 3-body collisions. This then can be used to factorize the system U- (or S-) matrix into reaction U- (or S-) matrices. Of course, this simplification is not essential for the existence of a system U-matrix; it only allows for easy visualization.

We now return to our problem. If there are M particles in the box, the overall wave function is contained in a 3M-dimensional finite configuration space; at fixed total energy the phase space of the system is also finite and has, say, N cells. Then the overall system S-matrix is N by N; it is sparse but not disconnected. Except for its size, it has all the same attributes as the S-matrix of a two-body system discussed above. It allows the definition of system eigenchannel states. Again, these states are time-reversal invariant, and are the only time-reversal invariant states. The remarks that the time-reversal invariant solutions are mathematically unstable made above for a two-body system thus apply also for a many-body system. (Since N is the volume of the phase space it actually is ridiculously inconceivable to construct a state with phase-related incoming waves in all N channels which would be needed for the time-reversal invariant state.)

The point of the mathematical instability of the time-reversal invariant solutions requires a precise demonstration. In the eigenchannel representation the S-matrix is diagonal with diagonal elements $e^{-2i\eta_n}$. In this representation the state vector of the given eigenchannel, n, is $\delta_{n,m}$. It has non-vanishing amplitudes in all components of the asymptotic state representation. Each action of the S-matrix generates the "outgoing" wave by multiplying each of the "incoming" wave components by the factor $e^{-2i\eta_n}$, common to all these components. The ratio of the amplitudes thus is not altered by the collision; the system is in a stationary state. If, however, only one more eigenchannel solution, say m, is admixed then "after" the collision the amplitude in channel c will be

$$b_c \;=\; a_{c,n}\, e^{-2i\eta_n} \;+\; a_{c,m}\, e^{-2i\eta_m} \quad . \tag{6}$$

Since in view of the orthogonality of the eigenchannels in general the ratio $a_{c,n}/a_{c,m}$ is different for the different channels c, the state after the collision is not an eigenchannel state. Furthermore, as long as $(\eta_n \;-\; \eta_m)/\pi$ is not a rational number, the system will never return to the state it occupied "before the first collision." Therefore, the Poincaré time then is infinite. Nonetheless, a time-reversed invariant state can be constructed by the prescription (1). Admixing further eigenchannel solutions does not change the situation in any qualitative manner. Of course, in that case there exist more relative phases, generally irrational multiples of π, between the contributing eigenchannel states; this then allows for greater variety of trajectories in the asymptotic-representation Hilbert space. This discussion thus provides the precise definition of quantum chaos: except for the case of being in a single eigenchannel state, every quantum system is chaotic unless all ratios of the eigenphases are rational numbers. From this follows that already a "small" system with a 2 by 2 S-matrix, thus having 2 eigenchannel states, according to Eq. (6) can exhibit quantum chaos. Furthermore, time-reversal invariance does not imply that the state is non-chaotic; on the other hand a non-chaotic state must exhibit time- reversal invariance. So, for example, a physical state time-symmetrized according to Eq. (1), can be, and in general will be, in a chaos state.

Concerning the rationality of the ratio $(\eta_n - \eta_m)/\pi$, this can happen in an N by N S-matrix if at all, then for 2 eigenchannels, and only by some accidental degeneracy. We have not been able to invent a non-trivial system exhibiting this characteristic in a non-accidental way, as we are dealing with systems above some inelastic thresholds. Besides, even an approximate Poincaré return, defined in some suitable manner, is thwarted because the Weyl states do "flow apart" in a time $1/\epsilon$, cf. Eq. (2), which is short compared with even any reasonable "quasi – Poincaré" time.

3 Dissipation

Having recognized that owing to the unstable nature of the time-reversal invariant states, in particular their non-return character, there is nothing left to distinguish them from a generic state. The question we now must address is what is the nature of the state the system evolves into, starting from some arbitrary "initial state." To answer that question we investigate, again for the case of a dilute gas, the change induced in the system by "the next collision." As explained in the previous section, the time evolution is governed by the (N by N) system U- or S-matrix.

Assume that before the considered collision, i.e., after the last collision, the amplitudes of the system wave function in the asymptotic representation are a_j, and, furthermore, we assume that the state is not an eigenchannel state. Then the amplitudes after the next collision are given by multiplication of the original amplitudes by the system S-matrix. Denoting the system S-matrix elements by R_{ij}, then the new amplitudes, $\bar{a}_j$, thus will be

$$\bar{a}_1 = (1 - R_{11})\, a_1 + R_{12}\, a_2 + R_{13}\, a_3 + \cdots \tag{7a}$$

$$\bar{a}_2 = R_{21}\, a_1 + (1 - R_{22})\, a_2 + R_{23}\, a_3 + \cdots \tag{7b}$$

$$\cdots$$

$$\bar{a}_j = R_{j1}\, a_1 \cdots + (1 - R_{jj})\, a_j \cdots + R_{jk}\, a_k + \cdots \tag{7c}$$

$$\cdots$$

$$\bar{a}_k = R_{k1}\, a_1 \cdots + R_{kj}\, a_j + \cdots + (1 - R_{kk})\, a_k + \cdots \tag{7d}$$

$$\cdots$$

Owing to the unitarity of the S-matrix there holds

$$\sum |a_j|^2 = \sum |\bar{a}_j|^2 = 1 \quad . \tag{8}$$

The elements R_{jk}, $j \neq k$, describe cross-flow of probability amplitudes between the channels j and k, the elements R_{jj} reflect the net in-(or out-)flow into channel j.

Take as the measure of pair-wise non-uniformity the expression

$$\Delta_{jk} = |a_j|^2 - |a_k|^2 \quad . \tag{9}$$

From (7c) and (7d) we compute the change in the non-uniformity ($\bar{\Delta}_{jk}$: after the collision)

$$\begin{aligned} \bar{\Delta}_{jk} - \Delta_{jk} &= \left(|\bar{a}_j|^2 - |\bar{a}_k|^2\right) - \left(|a_j|^2 - |a_k|^2\right) \\ &= -|R_{jk}|^2\, \Delta_{jk} + [F] \quad . \end{aligned} \tag{10}$$

Because of the negative sign on the right-hand side, Eq. (10) has the character of a damping term. Hence we have the important result that Δ_{jk} relaxes towards zero (see remark below). This is true for every pair, j, k. The other terms, denoted by $[F]$ in Eq. (10), are of the form $a_j^*\, a_k - a_j\, a_k^*$ and thus are phase-sensitive. These terms induce fluctuations in Δ_{jk}, which are damped by Eq. (10). Both the fluctuations and the relaxation can be followed by repeated matrix multiplication. (Note that the form of the damping term, including it being real, results from the time-reversal invariance of the S-matrix.) Furthermore, the terms $[F]$ are responsible for maintaining (unstably) the amplitude and phase relations between the channels in the eigenchannel solutions.

An important remark here is in order. Namely, it is at this point that the results of the previous section, in particular that the Poincaré time for chaotic quantum systems is infinite, are decisive. Without those results the statements of the above paragraph would be unsupported. One would have to rely on some assumptions like random phases to eliminate, or at least to decrease the influence of, the fluctuation inducing terms $[F]$; they otherwise could in effect provide the dominant influence, e.g., leading to macroscopically observable fluctuations.

We now discuss our result. Recall that the channels of the system S-matrix are the cells of the overall system phase space. Thus the amplitude a_j is directly the occupation amplitude for phase space cell j, and thus the occupation probability for that cell is $|a_j|^2$. Hence, even though the Hamiltonian is time-reversal invariant, the dynamics of the system tends to achieve equal *a posteriori* probability for the occupation of the energetically accessible phase space. This is simply the consequence of the "no return" character of the reaction, and of the non-zero value of some R_{jk}, together with the connectedness of the S-matrix. If the S-matrix should turn out to be disconnected, then the equalization would take place within each connected piece of the S-matrix. A fully disconnected S-matrix actually does not occur in nature; what does occur is that by virtue of the smallness of the relevant R_{jk}, some parts of the S-matrix are only weakly connected to the rest of the S-matrix. In that case the overall equalization of the occupation probabilities would be slowed down; the overall system very well might, and actually usually does, have a set of different relaxation time constants.

In summary: the central result of this discussion is that evidently quantum dynamics achieves directly a uniform occupation of the accessible phase space. Now recall that all results of statistical thermodynamics are arrived at by assuming axiomatically equal *a priori* occupation probability of all accessible phase space cells, and evaluating the resulting probability by counting the phase space cells. Our result shows that we have proven the correctness of that axiom for quantum dynamics. (Note that Eq. (10) concerns only the occupation probabilities, $|a_j|^2$; the amplitudes still may contain phase relations, which, however, has no importance for our result. A detailed discussion of this point will be given in a subsequent paper.) Hence, not only are the results of statistical thermodynamics correct, even more strongly: we have proven that statistical thermodynamics is a direct consequence of quantum physics. In particular, one of these consequences is the validity of the second law of thermodynamics; it arises as a direct consequence of the time-reversal invariance of the quantum physics Hamiltonian and the equations of motion derived from this Hamiltonian, which underlie the form and even the reality of the right-hand side of Eq. (10). At the same time this allows the definition of quantum entropy (which, however, we will not address here), and with it the definition of the arrow of time for non-equilibrium systems in quantum physics. No arrow of time can be defined for systems at equilibrium. In view of the fact that the first law of thermodynamics, being only the expression of energy conservation, is contained in quantum physics, the overall conclusion is that the field of thermodynamics is simply part of quantum physics.

Note that in this whole discussion the question of measurement did not arise and did not have to be addressed. Measurement evidently is irrelevant to the existence of dissipation. In particular, the well-known collapse of the wave function plays no role here. This is not to say that an analysis of the measurement process for a many-body system is of no interest; to the contrary, it is very worthwhile to give a careful discussion of that problem, in particular, in the context of the definition of the observables representing the microscopic thermodynamic variables. Simply, it lies outside of the frame of the present note.

To apply our results to nature, first note that no questions of general relativity, e.g., the expansion of the universe, have been addressed. Ignoring that aspect, we recall that the eigenchannels belong to isolated points in Hilbert space. Since one knows that some parts of nature are not on the eigenchannel points, no part of nature can escape equilibration. Finally, since for a (Weyl discretized!) N by N S-matrix (N is the total volume of the phase space of the universe) the number of eigenchannel states is N, while the total number of states is $N!$, the chances that a "New Universe" will land in an eigenchannel point, i.e., $(1/(N-1)!)$, seem to be negligibly small.

Acknowledgments

I would like to acknowledge many useful discussions about the concepts of the present paper with many colleagues, including H. Bers, S. Chandrasekhar, U. Fano, H. Fritsche, D. Mueller, Y. Nambu, D. Oxtoby, and R. Wald. I am particularly grateful for very helpful and stimulating discussions with P. Carruthers and especially with J. Rafelski, who in addition not only contributed essentially in clarifying my thinking but actually provided the initial stimulus which led to this work.

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